

Spin-triplet superconductivity due to antiferromagnetic spin-fluctuation in Sr_2RuO_4

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A mechanism leading to the spin-triplet superconductivity is proposed based on the antiferromagnetic spin fluctuation. The effects of anisotropy in spin fluctuation on the Cooper pairing and on the direction of \mathbf{d} vector are examined in the one-band Hubbard model with RPA approximation. The gap equations for the anisotropic case are derived and applied to Sr_2RuO_4 . It is found that a nesting property of the Fermi surface together with the anisotropy leads to the triplet superconductivity with the $\mathbf{d} = \hat{z}(\sin k_x \pm i \sin k_y)$, which is consistent with experiments.

74.20-z, 74.20Mn, 74.25Dw

Since the discovery of superconducting phase in Sr_2RuO_4 [1], much effort has been paid for understanding its exotic properties. Among several interesting natures, the most fascinating one is that it is a spin-triplet superconductor confirmed by NMR experiment [2]. While most superconductors found during several decades are singlet, the only exceptions were ^3He and UPt_3 . Therefore the fact that the triplet pairing is realized in Sr_2RuO_4 has attracted much attention. While UPt_3 , the second example of spin-triplet superconductor, has a complicated electronic structure, Sr_2RuO_4 has a rather simple electronic state [1]. Thus clarifying the microscopic mechanism of superconductivity in Sr_2RuO_4 is very important for understanding the triplet superconductors in general.

In ^3He , Cooper pairs are formed due to ferromagnetic spin fluctuations peaked at $\mathbf{q} = \mathbf{0}$ [3,4]. Therefore it is natural to expect the origin of the triplet pairing in Sr_2RuO_4 is also ferromagnetic spin fluctuation [5,6]. This assumption has been believed to be justified by NMR experiments [7–9]. However the recent neutron scattering experiment has shown that there exists a significant peak near $\mathbf{q}_0 = (\pm 2\pi/3, \pm 2\pi/3)$ and no sizable ferromagnetic spin fluctuation [10]. Thus it is difficult to assume that the spin fluctuation near \mathbf{q}_0 plays no role in the Cooper pairing in Sr_2RuO_4 . (In the following discussion we call this fluctuation as antiferromagnetic (AF) spin fluctuation, for simplicity.) However this AF fluctuation leads to the singlet superconductivity rather than

the triplet superconductivity as expected in analogy to high- T_c cuprates [5].

In this paper we propose a mechanism which gives the triplet pairing even if the spin fluctuation is AF. We find that the characteristic features of Sr_2RuO_4 are twofold: One is the anisotropy of the spin fluctuation found in NMR experiments [8,9], and the other is a nesting property with momentum \mathbf{q}_0 of the two-dimensional Fermi surface. We show that these two features explain the pairing in Sr_2RuO_4 .

In addition to the competition between singlet and triplet pairing, the direction of the \mathbf{d} vector, which is the order parameter of triplet superconductivity, is another interesting problem. We show that the anisotropy of the spin fluctuation also explains the experimental fact that the \mathbf{d} vector is parallel to the z -direction [2]. First we extend the RPA formulation to the case of anisotropic spin fluctuation. Using the obtained effective interactions, we investigate the most stable pairing based on the weak-coupling gap equations. When the spin fluctuation is isotropic, the so-called $d_{x^2-y^2}$ -wave pairing is the most stable. However when the anisotropy is increased, the state corresponding to $\hat{z}(\sin k_x \pm i \sin k_y)$, which is the prime candidate of Sr_2RuO_4 , becomes the most stable.

For the γ band which is one of the three bands in Sr_2RuO_4 [11], we assume a two-dimensional effective Hamiltonian

$$H = H_0 + \frac{I}{2N} \sum_{kk'q\sigma} c_{k\sigma}^\dagger c_{k'-\sigma}^\dagger c_{k'-q-\sigma} c_{k+q\sigma}, \quad (1)$$

where $c_{k\sigma}$ is the annihilation operator of an electron with momentum \mathbf{k} and spin σ . We consider only the on-site Coulomb repulsion, I , as in the previous studies of spin-fluctuation mechanism. Among the three bands, we consider the γ band consisting of the antibonding band of Ru $4d_{xy}$ and O $2p_\pi$ orbitals in this paper, because it has the largest density of states at Fermi energy and the superconductivity is considered to be realized predominantly in the γ band [12]. Although the spin fluctuation near \mathbf{q}_0 is understood from the nesting effect of α and β bands [5], we assume that the wave-number dependence of spin fluctuation is common in the three bands due to some interactions, such as spin-orbit couplings and/or Hund couplings. In the following calculation, we use the γ band. However the same discussions can be also applied to the α and β bands.

The anisotropy of spin fluctuation observed experimentally is implicitly included in the two-body Hamiltonian, H_0 . Our purpose is not to investigate the origin

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of anisotropy in details but to examine the role of the anisotropy to Cooper pairing. Therefore we introduce a phenomenological parameter α by

$$\chi_{(+-, 0)}(\mathbf{q}) = \alpha \chi_{(\uparrow\uparrow, 0)}(\mathbf{q}), \quad (2)$$

where $\chi_{(\uparrow\uparrow, 0)}(\mathbf{q})$ ($\chi_{(+-, 0)}(\mathbf{q})$) is the unperturbed static susceptibility of z axis (xy plane), which originates from H_0 . The parameter α represents the anisotropy of spin fluctuation and we take $\alpha \leq 1$ since NMR experiments show that $\chi_{(xx)} < \chi_{(zz)}$ [8,9].

Using this one-band model, we discuss the effective interactions between Cooper pairs due to spin fluctuations. Summation of bubble and ladder diagrams (i.e., RPA approximation) gives

$$\begin{aligned} H_{\text{int}} = & - \sum_{kk's} V_{\text{b.o}}(\mathbf{k} - \mathbf{k}') c_{ks}^\dagger c_{-ks}^\dagger c_{-k's} c_{k's} \\ & + \sum_{kk's} V_{\text{b.e}}(\mathbf{k} - \mathbf{k}') c_{ks}^\dagger c_{-k-s}^\dagger c_{-k'-s} c_{k's} \\ & - \sum_{kk's} V_{\text{lad}}(\mathbf{k} - \mathbf{k}') c_{ks}^\dagger c_{-k-s}^\dagger c_{-k's} c_{k'-s}, \end{aligned} \quad (3)$$

with

$$\begin{aligned} V_{\text{b.o}}(\mathbf{k} - \mathbf{k}') &= \frac{I}{N} \frac{(I/N) \chi_{(\uparrow\uparrow, 0)}(\mathbf{k} - \mathbf{k}')}{1 - (I/N)^2 \chi_{(\uparrow\uparrow, 0)}^2(\mathbf{k} - \mathbf{k}')}, \\ V_{\text{b.e}}(\mathbf{k} - \mathbf{k}') &= \frac{I}{N} \frac{(I/N)^2 \chi_{(\uparrow\uparrow, 0)}^2(\mathbf{k} - \mathbf{k}')}{1 - (I/N)^2 \chi_{(\uparrow\uparrow, 0)}^2(\mathbf{k} - \mathbf{k}')}, \\ V_{\text{lad}}(\mathbf{k} - \mathbf{k}') &= \frac{I}{N} \frac{(I/N) \chi_{(+-, 0)}(\mathbf{k} - \mathbf{k}')}{1 - (I/N) \chi_{(+-, 0)}(\mathbf{k} - \mathbf{k}')}. \end{aligned} \quad (4)$$

Here $V_{\text{b.o}}$ ($V_{\text{b.e}}$) comes from the summation of diagrams with odd (even) number of bubbles, and V_{lad} from the ladder diagrams. It is apparent that $V_{\text{b.o}}$ is between the electrons with equal spins while $V_{\text{b.e}}$ and V_{lad} are between those with the opposite spins.

It is straightforward to derive the gap equations in the anisotropic case, using the method developed by Leggett [13]. First we introduce the operators

$$t_k^{(0)} = \sum_{ss'} (\sigma_2)_{ss'} c_{-ks} c_{ks'}, \quad (5)$$

$$t_k^{(a)} = \sum_{ss'} (\sigma_2 \sigma_a)_{ss'} c_{-ks} c_{ks'}, \text{ for } a = 1, 2, 3, \quad (6)$$

where σ_a ($a = 1, 2, 3$) are Pauli matrices. The operator $t_k^{(0)}$ ($t_k^{(a)}$) corresponds to spin singlet (triplet) Cooper pairs. In terms of these operators, the effective interaction (3) can be rewritten as

$$\begin{aligned} H_{\text{int}} = & \frac{1}{4} \sum_{kk'} V_{\text{sin}}(\mathbf{k} - \mathbf{k}') t_k^{(0)\dagger} t_{k'}^{(0)} \\ & + \frac{1}{4} \sum_{kk'} \sum_{a=1}^3 V_{\text{tri}}^{(a)}(\mathbf{k} - \mathbf{k}') t_k^{(a)\dagger} t_{k'}^{(a)}, \end{aligned} \quad (7)$$

where

$$\begin{aligned} V_{\text{sin}}(\mathbf{k} - \mathbf{k}') &\equiv 2[V_{\text{b.e}}(\mathbf{k} - \mathbf{k}') + V_{\text{lad}}(\mathbf{k} - \mathbf{k}')], \\ V_{\text{tri}}^{(1)}(\mathbf{k} - \mathbf{k}') &= V_{\text{tri}}^{(2)}(\mathbf{k} - \mathbf{k}') \equiv -2V_{\text{b.o}}(\mathbf{k} - \mathbf{k}'), \\ V_{\text{tri}}^{(3)}(\mathbf{k} - \mathbf{k}') &\equiv 2[V_{\text{b.e}}(\mathbf{k} - \mathbf{k}') - V_{\text{lad}}(\mathbf{k} - \mathbf{k}')]. \end{aligned} \quad (8)$$

Since Sr_2RuO_4 has a long coherence length in ab plane, $\xi_{ab} \approx 660 \text{ \AA}$ [14], we use mean-field approximation to H_{int} . We restrict the discussion to unitary states because it is unrealistic to assume non-unitary states in Sr_2RuO_4 [15]. Requiring that there is no coexistence of singlet and triplet pairs, we obtain the gap equations

$$\begin{aligned} \Delta(\mathbf{k}) &= - \sum_{k'} V_{\text{sin}}(\mathbf{k} - \mathbf{k}') \Delta(\mathbf{k}') \Theta(E_{\text{sin}}(\mathbf{k}')), \\ d^{(a)}(\mathbf{k}) &= - \sum_{k'} V_{\text{tri}}^{(a)}(\mathbf{k} - \mathbf{k}') d^{(a)}(\mathbf{k}') \Theta(E_{\text{tri}}(\mathbf{k}')), \end{aligned} \quad (9)$$

where $\Theta(E) \equiv \frac{1}{2E} \tanh \frac{\beta E}{2}$, $E_{\text{sin}}^2(\mathbf{k}) = \xi_k^2 + \Delta(\mathbf{k}) \Delta^*(\mathbf{k})$, and $E_{\text{tri}}^2(\mathbf{k}) = \xi_k^2 + \mathbf{d}(\mathbf{k}) \cdot \mathbf{d}^*(\mathbf{k})$ with $\xi_k = \varepsilon_k - \mu$. The singlet and triplet order parameters are defined as $\Delta(\mathbf{k}) = -\frac{1}{2} \sum_{k'} V_{\text{sin}}(\mathbf{k} - \mathbf{k}') \langle t_{k'}^{(0)} \rangle$ and $d^{(a)}(\mathbf{k}) = -\frac{1}{2} \sum_{k'} V_{\text{tri}}^{(a)}(\mathbf{k} - \mathbf{k}') \langle t_{k'}^{(a)} \rangle$, respectively. Here $\mathbf{d}(\mathbf{k})$ is the so-called \mathbf{d} -vector for the triplet superconductivity.

In the system with the rotational symmetry in spin space, $\chi_{(\uparrow\uparrow, 0)}(\mathbf{q}) = \chi_{(+-, 0)}(\mathbf{q})$ is satisfied and thus the relation $V_{\text{b.o}} + V_{\text{b.e}} = V_{\text{lad}}$ holds. In this case, it is easy to see $V_{\text{tri}}^{(1)}(\mathbf{k} - \mathbf{k}') = V_{\text{tri}}^{(2)}(\mathbf{k} - \mathbf{k}') = V_{\text{tri}}^{(3)}(\mathbf{k} - \mathbf{k}')$.

On the other hand, the gap equation in Eq. (9) for the triplet pairing becomes dependent on the direction of the \mathbf{d} vector in the anisotropic case. It means that *\mathbf{d} vector has some preferred direction if the triplet pairs are formed by anisotropic spin fluctuations.* This is naturally understood because the \mathbf{d} vector is orthogonal to the spin direction of triplet Cooper pairs [16]. For the present case with $\chi_{(+-, 0)}(\mathbf{q}) < \chi_{(\uparrow\uparrow, 0)}(\mathbf{q})$ (i.e., $\alpha < 1$) which is applied to the Sr_2RuO_4 , we can see from Eq. (4) that $V_{\text{lad}}(\mathbf{k} - \mathbf{k}')$ is suppressed and the effective interaction $V_{\text{tri}}^{(3)}(\mathbf{k} - \mathbf{k}')$ approaches $V_{\text{sin}}(\mathbf{k} - \mathbf{k}')$. Consequently the triplet superconductivity with $d^{(3)}(\mathbf{k})$ (i.e., $\mathbf{d} \parallel \hat{\mathbf{z}}$) can be stabilized even due to the AF spin fluctuations.

In order to determine the symmetry of the superconducting order parameter, we have to take account of their sign change along the Fermi surface. For the high- T_c superconductors, the AF spin fluctuation with momentum (π, π) stabilizes the singlet $d_{x^2-y^2}$ -wave superconductivity. In that case, the singlet order parameters $\Delta(\mathbf{k}')$ with $\mathbf{k}' = (\pi, 0)$ and $\Delta(\mathbf{k})$ with $\mathbf{k} = (0, \pi)$ have the opposite sign, so that the gap equation in (9) is satisfied with $V_{\text{sin}}(\pi, \pi) > 0$.

For Sr_2RuO_4 we consider that a kind of *nesting* property of the Fermi surface plays an important role. This is the second point of our mechanism. Figure 1 shows a schematic Fermi surface for the γ band. Since the AF fluctuation in Sr_2RuO_4 has momentum \mathbf{q}_0 , the Fermi surface is also shifted by $(2\pi/3, 2\pi/3)$ in Fig. 1. It is apparent that some part of the shifted Fermi surface overlaps

with the original Fermi surface with modulo 2π . In analogy to the case of high- T_c superconductivity, if the superconducting order parameters have the opposite sign on these overlapping portions of the Fermi surface, the gap equation is satisfied with $V_{\text{tri}}^{(a)}(2\pi/3, 2\pi/3) > 0$. From Fig. 1, it is natural to consider the p-wave pairing instead of the singlet $d_{x^2-y^2}$ -wave pairing.

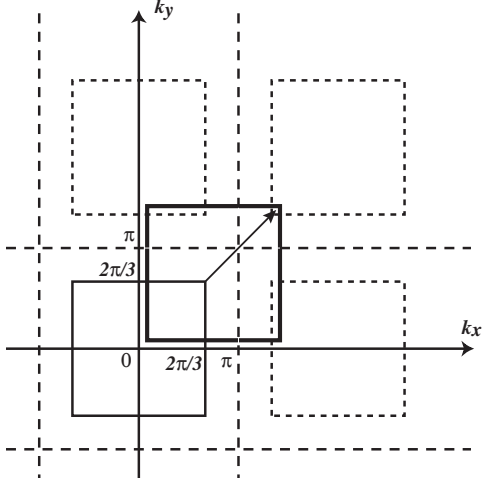


FIG. 1. A schematic Fermi surface for the γ band of Sr_2RuO_4 . In order to show the nesting property, the Fermi surface shifted by the AF wave number, \mathbf{q}_0 , is also shown by the solid line. The thin dashed lines indicate the Fermi surfaces in the extended Brillouin zone.

In order to clarify this point quantitatively, we compare various kinds of anisotropic superconductivity using the effective interaction and the simplified Fermi surface. Near the transition temperature T_c , we rewrite the gap equations as

$$\phi(\mathbf{k}) = - \sum_{\mathbf{k}'} V_\phi(\mathbf{k} - \mathbf{k}') \phi(\mathbf{k}') \frac{1}{2\xi_{k'}} \tanh \frac{\beta_c \xi_{k'}}{2}, \quad (10)$$

where $\phi(\mathbf{k})$ represents one of the order parameters $\Delta(\mathbf{k})$ or $d^{(a)}(\mathbf{k})$, and V_ϕ is determined from Eqs. (8) depending on ϕ . In the weak coupling approximation, T_c is obtained as

$$k_B T_c = 1.13 \hbar v_F k_c \exp \left[- \frac{1}{N(0) \langle \langle V_\phi \rangle \rangle_{FS}} \right], \quad (11)$$

where v_F , k_c and $N(0)$ are the Fermi velocity, cut-off of the wave number, and the density of states at the Fermi energy, respectively. $\langle \langle V_\phi \rangle \rangle_{FS}$ means the average over the Fermi surface,

$$\langle \langle V_\phi \rangle \rangle_{FS} \equiv - \frac{\int_{FS} d\mathbf{k} \int_{FS} d\mathbf{k}' V_\phi(\mathbf{k} - \mathbf{k}') \phi(\mathbf{k}) \phi(\mathbf{k}')}{\left[\int_{FS} d\mathbf{k}' \right] \int_{FS} d\mathbf{k} \phi^2(\mathbf{k})}. \quad (12)$$

We identify that the order parameter which gives the largest $N(0) \langle \langle V_\phi \rangle \rangle_{FS}$ is realized.

For Sr_2RuO_4 we choose order parameters $\phi(\mathbf{k})$ as follows

$$\begin{aligned} \phi_1(\mathbf{k}) &= \cos k_x + \cos k_y, \\ \phi_2(\mathbf{k}) &= \cos k_x - \cos k_y, \\ \phi_3(\mathbf{k}) &= \sin k_x \sin k_y, \\ \phi_4(\mathbf{k}) &= \sin k_x, (\hat{\mathbf{d}} \perp \hat{\mathbf{z}}), \\ \phi_5(\mathbf{k}) &= \sin k_x, (\hat{\mathbf{d}} \parallel \hat{\mathbf{z}}), \end{aligned} \quad (13)$$

where $\phi_1 \sim \phi_3$ correspond to singlet pairings, and ϕ_4, ϕ_5 to triplet pairings, respectively. The most probable candidate for Sr_2RuO_4 is $\hat{\mathbf{z}}(\sin k_x \pm i \sin k_y)$ which is equivalent to ϕ_5 just below T_c , because the gap equation (10) for $\sin k_x \pm i \sin k_y$ is exactly same as that for ϕ_5 . If $N(0) \langle \langle V_{\phi_5} \rangle \rangle_{FS}$ is the largest, we expect that the order parameter $\mathbf{d}(\mathbf{k}) = \hat{\mathbf{z}}(\sin k_x \pm i \sin k_y)$ is realized, because near zero temperature it acquires a larger energy gap than ϕ_5 .

To emphasize the characteristic feature of the nesting, we assume the simplified Fermi surface as shown in Fig. 1. For the \mathbf{q} dependence of $\chi_{(\uparrow\uparrow, 0)}(\mathbf{q})$ with a maximum at \mathbf{q}_0 , we use the susceptibility obtained in the LDA calculation [5], and fix $S(0) = 0.8$ with $S(\mathbf{q}) \equiv \frac{1}{N} \chi_{(\uparrow\uparrow, 0)}(\mathbf{q})$. We regard $S(\mathbf{q}_0)$ as a phenomenological parameter.

Figure 2 shows the α dependence of $N(0) \langle \langle V_{\phi_n} \rangle \rangle_{FS}$ ($n = 1 \sim 5$) for $S(\mathbf{q}_0) = 0.95$. We examined various choices of $S(\mathbf{q}_0)$ from 0.90 to 0.99 to find that the results do not change qualitatively. When the anisotropy is weak ($\alpha \sim 1$), the singlet $d_{x^2-y^2}$ -wave superconductivity, ϕ_2 , is stabilized. On the other hand, when α is small, the order parameter ϕ_5 is stabilized which is consistent with experiments.

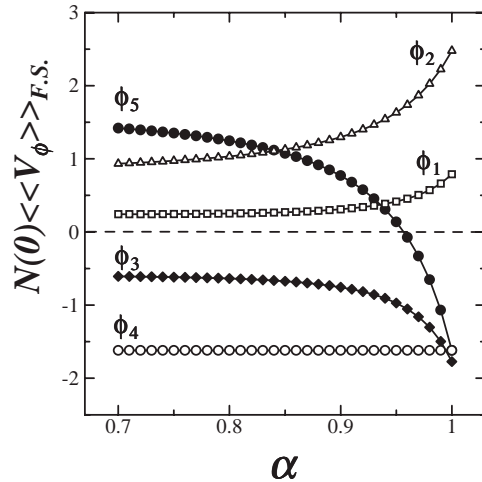


FIG. 2. The dependence of the anisotropy parameter, α , of $N(0) \langle \langle V_{\phi_n} \rangle \rangle_{FS}$ ($n = 1 \sim 5$) for $S(\mathbf{q}_0) = 0.95$.

The phase diagram as a function of α and $S(\mathbf{q}_0)$ is determined by examining various values of $S(\mathbf{q}_0)$. Because it is unphysical to assume that $S(\mathbf{q}_0)$ is very close to 1, we show the results up to $S(\mathbf{q}_0) = 0.99$ in Fig. 3. When the spin fluctuation is isotropic (i.e., $\alpha = 1$), the singlet $d_{x^2-y^2}$ -wave superconductivity, $\cos k_x - \cos k_y$, is the most stable pairing. This is consistent with the previous studies [5]. However we find a fairly large parameter

region where the state corresponding to $\hat{z}(\sin k_x \pm i \sin k_y)$ is realized.

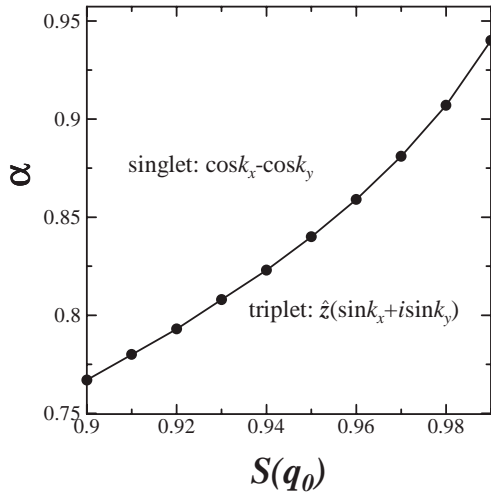


FIG. 3. Phase diagram as a function of the anisotropy parameter, α , and $S(q_0)$ which is the maximum of $S(\mathbf{q}) = (I/N)\chi_{(\uparrow\uparrow, 0)}(\mathbf{q})$, with $\mathbf{q}_0 = (\pm 2\pi/3, \pm 2\pi/3)$.

Finally we discuss the competition between the singlet $\cos k_x - \cos k_y$ pairing and the triplet $\hat{z}(\sin k_x \pm i \sin k_y)$ pairing in terms of the effective interaction and the nesting property. From the explicit form of V_{ϕ_n} for $n = 2$ and 5 , we can see that a relation $V_{\phi_2} \geq V_{\phi_5}$ is satisfied. Therefore if we consider only the magnitude of the effective interaction, the singlet pairing is favorable. However the nesting property favors the triplet pairing. Let us assume that V_{ϕ_n} is enhanced very strongly by the AF fluctuation and approximated as

$$V_{\phi_n}(\mathbf{q}) = \frac{I}{N} A_n \hat{\delta}(q_x \pm 2\pi/3) \hat{\delta}(q_y \pm 2\pi/3), \quad (14)$$

with $\hat{\delta}$ being the δ function with modulo 2π . Using this approximated form of V_{ϕ_n} ($n = 2$ and 5), we obtain

$$\begin{aligned} N(0)\langle\langle V_{\phi_2} \rangle\rangle_{FS} &= [-2.79 \times 10^{-2} \delta(0) + 4.91 \times 10^{-2}] A_2, \\ N(0)\langle\langle V_{\phi_5} \rangle\rangle_{FS} &= [4.24 \times 10^{-2} \delta(0) + 5.06 \times 10^{-2}] A_5. \end{aligned}$$

This estimation shows that the $\hat{z}(\sin k_x \pm i \sin k_y)$ pairing utilizes the peak of $\chi_{(\uparrow\uparrow, 0)}(\mathbf{q})$ at \mathbf{q}_0 more effectively than $\cos k_x - \cos k_y$ pairing does. Therefore, even if $A_2 > A_5$, the triplet pair can be stabilized.

In determining the phase diagram in Fig. 3, we have assumed simple functional forms of the order parameters, $\phi_n(\mathbf{k})$. For the detailed calculations, it will be necessary to optimize the \mathbf{k} -dependence of $\phi_n(\mathbf{k})$. However the global feature of the phase diagram will not change.

In summary, we have generalized the RPA formulation of the effective interaction due to the spin fluctuations and derived gap equations including the anisotropic case. We have shown that the state corresponding to $\hat{z}(\sin k_x \pm i \sin k_y)$ becomes the most stable even if the AF spin fluctuation is dominant, when the anisotropy is strong

enough and the nesting property of the Fermi surface is present. Although the nesting for the actual Fermi surface will be weaker than what we assumed here, it is reasonable to think that our mechanism is the most promising one as far as the AF fluctuation is dominant.

In this paper we have investigated the pairing in the γ band. However it is straightforward to consider the other bands (α and β bands) in Sr_2RuO_4 . Since the nesting property will be comparable or even stronger for these bands than for the γ band, we expect the same mechanism for triplet superconductivity for α and β bands even if the γ band does not have the peak near \mathbf{q}_0 .

It is reported that Sr_2RuO_4 has exotic property called as *3K phase* [17] when Ru metal is embedded in the single crystal. We speculate that the enhancement of T_c is due to the increase of the anisotropy (i.e., decrease of α) near the interface region between Sr_2RuO_4 and Ru metal. We consider that to investigate the origin of the anisotropy is very important both for understanding the superconductivity and for finding the new exotic phenomena.

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